

=&gt; d his ful

(FILE 'HOME' ENTERED AT 11:15:14 ON 23 MAR 2006)

FILE 'REGISTRY' ENTERED AT 11:15:54 ON 23 MAR 2006

L1 STR

L2 0 SEA SSS SAM L1

L3 7 SEA SSS FUL L1

*7 comps from Reg. for Str. I*

FILE 'HCAPLUS' ENTERED AT 11:29:40 ON 23 MAR 2006

L4 6 SEA ABB=ON L3

*6 cits from CAPLUS for Str. I*

FILE 'REGISTRY' ENTERED AT 11:30:03 ON 23 MAR 2006

L5 STR

L6 34 SEA SSS SAM L5

FILE 'HCAPLUS' ENTERED AT 11:37:34 ON 23 MAR 2006

L7 50 SEA ABB=ON L6

FILE 'REGISTRY' ENTERED AT 11:41:07 ON 23 MAR 2006

L8 813 SEA SSS FUL L5

*813 comps from Reg. for Str. II*

FILE 'HCAPLUS' ENTERED AT 11:41:16 ON 23 MAR 2006

L9 1374 SEA ABB=ON L8

FILE 'REGISTRY' ENTERED AT 11:43:58 ON 23 MAR 2006

L10 STR L5

L11 STR L5

L12 29 SEA SSS SAM L11

FILE 'HCAPLUS' ENTERED AT 11:54:40 ON 23 MAR 2006

L13 486 SEA ABB=ON L8 (L) RACT+ALL/RL

L14 2 SEA ABB=ON L13 AND L4

L15 6 SEA ABB=ON L4 OR L14

*486 cits for Str. III from CAPLUS.  
Last (earliest) 10 cits are included  
here with.*

FILE 'BEILSTEIN' ENTERED AT 12:00:51 ON 23 MAR 2006

L16 0 SEA SSS SAM L1

FILE 'MARPAT' ENTERED AT 12:01:42 ON 23 MAR 2006

FILE 'REGISTRY' ENTERED AT 12:02:45 ON 23 MAR 2006

L17 STR L1

FILE 'BEILSTEIN' ENTERED AT 12:04:22 ON 23 MAR 2006

L18 0 SEA SSS SAM L17

L19 4 SEA SSS FUL L17

L20 4 SEA ABB=ON L19/COM

L21 4 SEA ABB=ON L20 NOT L3

*4 cits from Beilstein*

FILE 'HCAPLUS' ENTERED AT 12:09:55 ON 23 MAR 2006

FILE 'USPATFULL' ENTERED AT 12:12:37 ON 23 MAR 2006

L22 1 SEA ABB=ON L3

L23 0 SEA ABB=ON L22 NOT L4

*0 cits from USPatfull that would  
be unique*

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file

*Structures X and XI would be included in above results since*

Searched by Mary Jane Ruhl

Ext. 22524

Page 25

*Those searches were more generic.*

provided by InfoChem.

STRUCTURE FILE UPDATES: 21 MAR 2006 HIGHEST RN 877591-95-2  
DICTIONARY FILE UPDATES: 21 MAR 2006 HIGHEST RN 877591-95-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

#### FILE HCAPLUS

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FILE COVERS 1907 - 23 Mar 2006 VOL 144 ISS 13  
FILE LAST UPDATED: 22 Mar 2006 (20060322/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

FILE BEILSTEIN  
FILE LAST UPDATED ON MARCH 15, 2006

FILE COVERS 1771 TO 2006.  
**FILE CONTAINS 9,516,393 SUBSTANCES**

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed

immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 144 ISS 12 (20060317/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2006035965	16	FEB	2006
DE	102004030305	12	JAN	2006
EP	1614691	11	JAN	2006
JP	2006008639	12	JAN	2006
WO	2006012333	02	FEB	2006
GB	2415429	28	DEC	2005
FR	2873371	27	JAN	2006
RU	2267521	10	JAN	2006
CA	2472818	30	DEC	2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 23 Mar 2006 (20060323/PD)

FILE LAST UPDATED: 23 Mar 2006 (20060323/ED)

HIGHEST GRANTED PATENT NUMBER: US7017190

HIGHEST APPLICATION PUBLICATION NUMBER: US2006064792

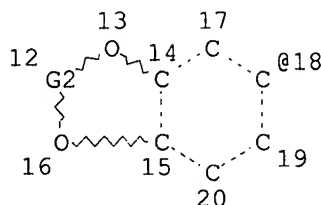
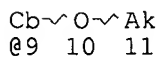
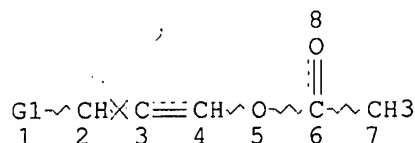
CA INDEXING IS CURRENT THROUGH 23 Mar 2006 (20060323/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 23 Mar 2006 (20060323/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2006

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2006

=> d que stat l4  
 l4 . STR



VAR G1=9/18  
 REP G2=(1-2) CH2  
 NODE ATTRIBUTES:  
 CONNECT IS E1 RC AT 11  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS MCY UNS AT 9  
 GGCAT IS LOC AT 11  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS E6 C AT 9

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE  
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 L4 6 SEA FILE=HCAPLUS ABB=ON L3

=> d ibib abs hitstr l4 1-6

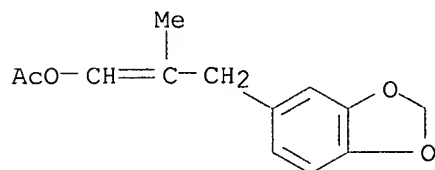
L4 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1023440 HCAPLUS  
 DOCUMENT NUMBER: 143:326081  
 TITLE: Process for preparation of 1-alkoxy-3-phenylpropene derivatives  
 INVENTOR(S): Shirai, Masashi; Sadaike, Shinichiro; Furuya, Toshio; Yoshida, Yoshihiro  
 PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005255632	A2	20050922	JP 2004-70490	20040312
PRIORITY APPLN. INFO.:			JP 2004-70490	20040312

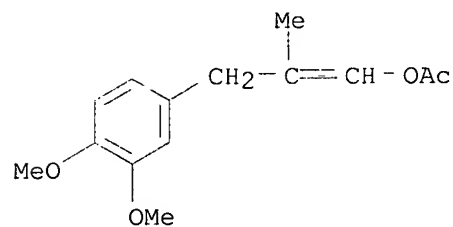
OTHER SOURCE(S): CASREACT 143:326081; MARPAT 143:326081

AB This invention pertains to a method for producing 1-alkoxy-3-phenylpropene derivs. which comprises reacting a alkoxybenzene compound with an  $\alpha, \beta$ -unsatd. aldehyde compound and an acid anhydride compound in the presence of a catalyst. The catalyst is triflate or halide of group 11-13 elements, Sn, or lanthanides. For example, anisole was reacted with methacrolein and acetic anhydride in the presence of  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  to give 1-acetoxy-2-methyl-3-(4-methoxyphenyl)propene (91.9%).

IT 714237-82-8P 714237-84-0P  
 ' RE: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (preparation of 1-alkoxy-3-phenylpropene derivs.)  
 RN 714237-82-8 HCAPLUS  
 CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate (9CI) (CA  
 INDEX NAME)



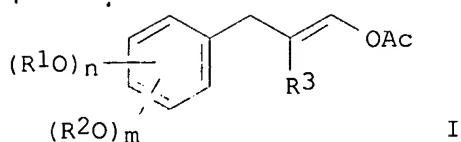
RN 714237-84-0 HCAPLUS  
 CN 1-Propen-1-ol, 3-(3,4-dimethoxyphenyl)-2-methyl-, acetate (9CI) (CA INDEX  
 NAME)



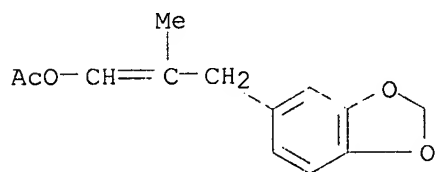
L4 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:979098 HCAPLUS  
 DOCUMENT NUMBER: 143:286173  
 TITLE: Preparation of 1-acetoxy-2,3-disubstituted propenes  
 from alkoxybenzenes and 2-substituted  
 1,3-diacetoxypropenes  
 INVENTOR(S): Shirai, Masashi; Yoshida, Yoshihiro; Furuya, Toshio;  
 Sadaike, Shinichiro  
 PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005239619	A2	20050908	JP 2004-50732	20040226
PRIORITY APPLN. INFO.:			JP 2004-50732	20040226
OTHER SOURCE(S):	MARPAT	143:286173		

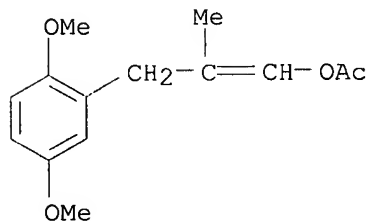
GI



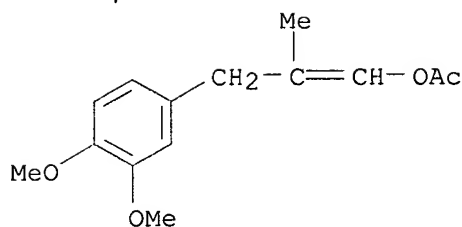
- AB 1-Acetoxy-2,3-disubstituted propenes I (R1, R2 = C1-4 alkyl; R1R2 may be linked to form OCH2O, OCH2CH2O; m = 0-4; n = 1-5) or their regioisomers are prepared by treatment of the corresponding alkoxybenzenes with AcOCH2CR3:CHOAc (R3 = C1-10 alkyl) or their regioisomers in the presence of catalysts containing B halides, Group 11 element triflates, Group 12 element halides, and/or triflates or halides of Ti, Sn, or lanthanoid element with atomic number 57-71. Thus, 1,2-methylenedioxybenzene was treated with 1,3-diacetoxy-2-methylpropene and BF3 etherate at 40° for 3 h to give 80.8% 1-acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene.
- IT **714237-82-8P**, 1-Acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene **714237-83-9P**, 1-Acetoxy-2-methyl-3-(2,5-dimethoxyphenyl)propene **714237-84-0P**, 1-Acetoxy-2-methyl-3-(3,4-dimethoxyphenyl)propene  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of acetoxypropenes from alkoxybenzenes and diacetoxypropenes with triflates or halides as catalysts)
- RN 714237-82-8 HCAPLUS
- CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



- RN 714237-83-9 HCAPLUS
- CN 1-Propen-1-ol, 3-(2,5-dimethoxyphenyl)-2-methyl-, acetate (9CI) (CA INDEX NAME)

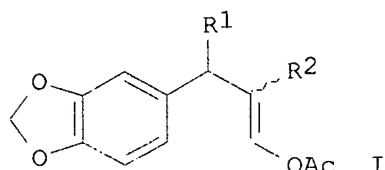


- RN 714237-84-0 HCAPLUS
- CN 1-Propen-1-ol, 3-(3,4-dimethoxyphenyl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:975885 HCAPLUS  
 DOCUMENT NUMBER: 143:248372  
 TITLE: Preparation of 1-acetoxy-3-(3,4-methylenedioxyphenyl)propenes  
 INVENTOR(S): Nishino, Shigeyoshi; Shirai, Masashi; Yoshida, Yoshihiro; Furuya, Toshio; Sadaike, Shinichiro  
 PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

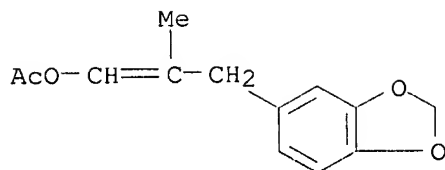
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005239620	A2	20050908	JP 2004-50733	20040226
PRIORITY APPLN. INFO.:			JP 2004-50733	20040226
OTHER SOURCE(S):	MARPAT 143:248372			
GI				



AB Title compds. I (R1, R2 = H, C1-10 alkyl; R1R2 may form ring) are prepared by treatment of 1,2-methylenedioxybenzene (II) with CHR1:CR2CH(OAc)2 (R1, R2 = same as above) in the presence of H2SO4 and/or sulfonic acids. Thus, II was treated with 3,3-diacetoxy-2-methylpropene in the presence of H2SO4 and purified to give 55% 1-acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene.

IT **714237-82-8P**, 1-Acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of acetoxy(methylenedioxyphenyl)propenes by Friedel-Crafts reaction of methylenedioxybenzene with alkenylidene diacetates in the presence of H2SO4 or sulfonic acid catalysts)

RN 714237-82-8 HCAPLUS  
 CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:369253 HCAPLUS

DOCUMENT NUMBER: 142:397314

TITLE: Short-chain enol esters as odoriferous substance precursors for cosmetic and cleaning agents

INVENTOR(S): Eh, Marcus; Panten, Johannes; Bertram, Heinz-Juergen

PATENT ASSIGNEE(S): Symrise GmbH & Co. Kg, Germany

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037243	A1	20050428	WO 2004-EP52520	20041013
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10348062	A1	20050519	DE 2003-10348062	20031016

PRIORITY APPLN. INFO.:

DE 2003-10348062 A 20031016

OTHER SOURCE(S): MARPAT 142:397314

AB The invention relates to the use of a compound of formula R2-CO-O-R1 wherein R1 represents the radical (a) of the enol form of an aldehyde comprising a min. of 6 C atoms, or (b) a ketone comprising a min. of 10 C atoms, and R2 represents a (a) branched or linear C1-4 alkyl group or (b) a branched or linear C2-4 alkylene group, as an odoriferous substance precursor. Enol esters can be added to perfume oils; the perfume oil can be adsorbed onto a carrier, microencapsulated, spray-dried, or obtained as inclusion complex or an extrudate. Thus series of enol esters were prepared; their storage stability and odorant effect was evaluated also in soaps and hair preps.

IT 849802-26-2P 849802-50-2P

RL: COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(short-chain enol esters as odoriferous substance precursors for cosmetic and cleaning agents)

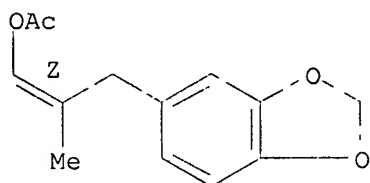
RN 849802-26-2 HCAPLUS

CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate, (1Z)- (9CI)



(CA INDEX NAME)

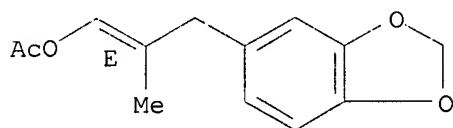
Double bond geometry as shown.



RN 849802-50-2 HCAPLUS

CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate, (1E)- (9CI)  
(CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:534188 HCAPLUS

DOCUMENT NUMBER: 141:88924

TITLE: Process for the production of 1-acetoxy-3-phenylpropenes

INVENTOR(S): Shirai, Masashi; Yoshida, Yoshihiro; Sadaike, Shinichiro

PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

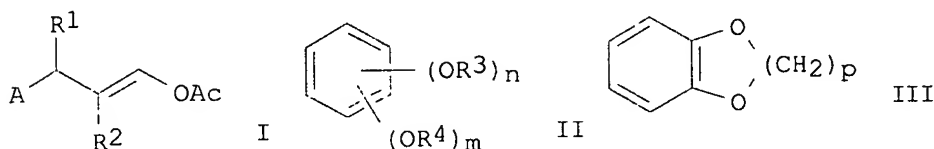
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054997	A1	20040701	WO 2003-JP16277	20031218
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003289432	A1	20040709	AU 2003-289432	20031218
EP 1574509	A1	20050914	EP 2003-780907	20031218
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

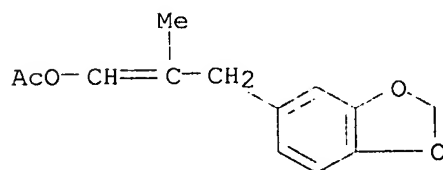
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 EP 1609775 A2 20051228 EP 2005-14610 20031218  
 EP 1609775 A3 20060118  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 CN 1738811 A 20060222 CN 2003-80108657 20031218  
 US 2006004213 A1 20060105 US 2005-155971 20050617  
 NO 2005003741 A 20040621 NO 2005-3741 20050804  
 PRIORITY APPLN. INFO.: JP 2002-367031 A 20021218  
 JP 2003-69733 A 20030314  
 JP 2003-316336 A 20030909  
 EP 2003-780907 A3 20031218  
 WO 2003-JP16277 W 20031218  
 OTHER SOURCE(S): CASREACT 141:88924; MARPAT 141:88924  
 GI



AB Title compds. I [wherein R1, R2 = independently H, alkyl; or R1R2 = cyclyl; A = (un)substituted Ph corresponding to II or III] can be produced by reacting a benzene compound II or III (R3, R4 = alkyl; m = 0-4; n = 1-5; p = 1-2) with an alkenylidene diacetate HC(R1)=C(R2)CH(OAc)2 in the presence of a catalyst comprising (a) a boron halide, (b) a triflate of a group 11 element, (c) a halide of a group 12 element, and (d) at least one member selected from among triflates and halides of tin and elements of atomic nos. of 58 and 66 to 71. For example, reaction of 1,2-methylenedioxybenzene with 3,3-diacetoxy-2-methylpropene using (di-Et ether)trifluoroborane as catalyst in AcOEt, gave 1-acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene in 88% yield.

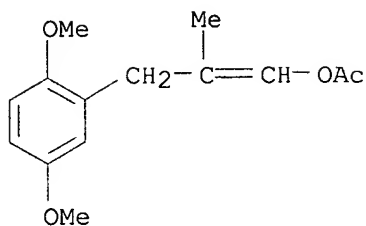
IT 714237-82-8P, 1-Acetoxy-2-methyl-3-(3,4-methylenedioxyphenyl)propene 714237-83-9P, 1-Acetoxy-2-methyl-3-(2,5-dimethoxyphenyl)propene 714237-84-0P, 1-Acetoxy-2-methyl-3-(3,4-dimethoxyphenyl)propene 714237-85-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of 1-acetoxy-3-phenylpropenes by using triflates of group IB element or halides of group IIB element as catalysts)

RN 714237-82-8 HCAPLUS  
 CN 1-Propen-1-ol, 3-(1,3-benzodioxol-5-yl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



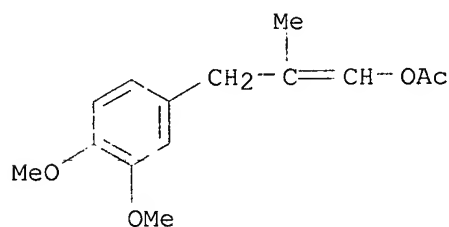
RN 714237-83-9 HCAPLUS

CN 1-Propen-1-ol, 3-(2,5-dimethoxyphenyl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



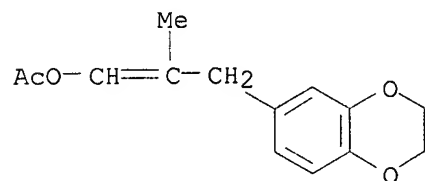
RN 714237-84-0 HCAPLUS

CN 1-Propen-1-ol, 3-(3,4-dimethoxyphenyl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



RN 714237-85-1 HCAPLUS

CN 1-Propen-1-ol, 3-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-methyl-, acetate (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1963:454653 HCAPLUS

DOCUMENT NUMBER: 59:54653

ORIGINAL REFERENCE NO.: 59:9900d-h,9901a

TITLE: Phenyl-substituted alkanals

INVENTOR(S): Scriabine, Igor

PATENT ASSIGNEE(S): Rhone-Poulenc S. A.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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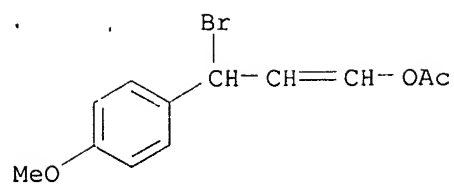
DE 1145161	19630314	DE 1958-S59254	19580731
PRIORITY APPLN. INFO.:		FR	19570801

AB Aryl compds. condense with  $\alpha$ -unsatd. aldehydes or their diacyl derivs. in the presence of  $\text{TiCl}_4$  and  $\text{BF}_3$  at  $-30$  to  $+20^\circ$  to give p-RC6H4CHR'CHR''-CHO (I). To cumene 52,  $\text{TiCl}_4$  19, and  $\text{BF}_3\cdot\text{Et}_2\text{O}$  0.55 at  $-10^\circ$  was added a solution of  $\alpha$ -methacrolein 7 in cumene 13. After 10 min. at  $-10^\circ$  the mixture was poured over ice 100 and concentrated  $\text{HCl}$  10. The organic layer was separated, washed with 5%  $\text{NaHCO}_2$ , dried over  $\text{MgSO}_4$ , and distilled to yield 6.68 parts I ( $R = \text{iso-Pr}$ ,  $R' = \text{H}$ ,  $R'' = \text{Me}$ ), b1  $92^\circ$  (semicarbazone m.  $170^\circ$ ). Substitution of 0.8 part  $\text{BF}_3\cdot 2\text{HOAc}$  for  $\text{BF}_3\cdot\text{Et}_2\text{O}$  in the reaction gave 5.51 parts of the same product. Similarly were prepared I (phenyl compound and parts, parts  $\text{TiCl}_4$ , parts  $\text{BF}_3\cdot\text{Et}_2\text{O}$ , aldehyde and parts, reaction temperature,  $R$ ,  $R'$ ,  $R''$ , and % yield of product given): toluene 147.2, 19, 0.6, acrolein 6,  $-27^\circ$ , Me, H, H, 6.1 (b1.5  $92-3^\circ$ , n30D 1.5171); cumene 384, 38, 1.3, acrolein 12,  $-30^\circ$ , iso-Pr, H, H, 13.4 (b0.5  $89-92^\circ$ , n25D 1.5111). Condensation of phenyl compds. (II) with alkenylidene diacetates  $R'\text{CH}:\text{CR}''\text{CH}(\text{OAc})_2$  (III) gave arylalkenyl acetates p-RC6H4CHR'CHR''CH2OAc (IV), which were hydrolyzed to I ( $R$ ,  $R'$ ,  $R''$ , parts II, parts  $\text{TiCl}_4$ , parts  $\text{BF}_3\cdot\text{Et}_2\text{O}$ , parts III, reaction time and temperature, yield and properties of IV, yield and (properties) of I, properties of their 2,4-dinitrophenylhydrazones (V) and semicarbazones (VI) given: iso-Pr, H, H, 650, 211, 3, 158, 140 min. at  $-10^\circ$ , 182.7 (b0.5  $101-3^\circ$ , n25D 1.5115), - (b0.9  $90-1^\circ$ ), -, VI m.  $148^\circ$ ; iso-Pr, H, Me, 647, 211, 3, 172, 140 min. at  $-10^\circ$ , 206 (b0.8  $101^\circ$ , d25 0.9813, n25D 1.5007), 138.3 (b0.6  $89^\circ$ ), -, VI m.  $170^\circ$ ; iso-Pr, Me, H, 650, 211, 3, 172, 140 min. at  $-10^\circ$ , 84 (b0.5  $107-10^\circ$ ), - (b0.5  $89-91^\circ$ ), V m.  $118-20^\circ$ , VI m.  $131-2^\circ$ ; iso-Pr, Et, Me, 130, 56.5, 0.5, 40, 140 min. at  $-10^\circ$ , 24.4 (b0.8  $114-15^\circ$ , n20D 1.5100), 16 (b0.9  $104-5^\circ$ ), V m.  $169-9.5^\circ$ , -; Me, Me, H, 80, 26, 0.5, 17.2, 140 min. at  $-10^\circ$ , 11.4 (b0.75,  $104-5^\circ$ ), - (b0.9  $110.5-11.5^\circ$ ), V m.  $106-9^\circ$ , VI m.  $78-81^\circ$  (p-nitrophenylhydrazone m.  $110-10.5^\circ$ ); H, H, H, 240, 82, 1.25, 63.2, 40 min. at  $6^\circ$ , 24.9 (b0.1  $85^\circ$ , n25D 1.5165), - (b12  $101^\circ$ , n21D 1.5190), -, VI m.  $127^\circ$ ; H, H, Me, 240, 82, 1.25, 68.8, 40 min. at  $6^\circ$ , 23.6 (b0.6  $90-2^\circ$ , n24D 1.5140), - (b6  $92^\circ$ , n24D 1.5087), V m.  $119^\circ$ , VI m.  $123^\circ$ ; H, H, Et, 240, 82, 1.25, 74.5, 40 min. at  $6^\circ$ , 29.2 (b0.9  $90-2^\circ$ , n24D 1.5105), - (b10  $104.5^\circ$ , n26D 1.5063), V m.  $116.5^\circ$ , -; H, H, iso-Pr, 240, 82, 1.25, 80, 40 min. at  $6^\circ$ , 17.5 (b0.5  $96.7^\circ$ , n24D 1.5060), - (b10.5  $120.5^\circ$ , n28D 1.5020), V m.  $143-4^\circ$ , -; Me, H, Et, 260, 85, 1.2, 74.5, 160 min. at  $-10^\circ$ , 67 (b2  $125-6^\circ$ , n31D 1.5090), 91% (b0.5  $86-6.5^\circ$ , n31D 1.5070, odor like cyclamal), V m.  $118-19^\circ$ , VI m.  $125-6^\circ$ ; Et, H, Et, 295, 85, 1.2, 74.5, 160 min. at  $-10^\circ$ , 65.5 (b1.3  $113-14^\circ$ , n32D 1.5075), 92% (b1  $98-9^\circ$ , n26D 1.5072), -, VI m.  $82-3^\circ$ ; iso-Pr, H, Et, 325, 85, 1.2, 74.5, 160 min. at  $-10^\circ$ , 57.8 (b1  $120^\circ$ , n25D 1.5060), 89% (b0.5  $94^\circ$ , n28.3D 1.5010), V m.  $98-9^\circ$ , -; MeO, H, H, 116, 43, 0.62, 31, 160 min. at  $-10^\circ$ , 35 (b1  $113-16^\circ$ , n25D 1.5245), 86% (b1  $82-4^\circ$ , n25D 1.5257), -, VI m.  $138^\circ$ . I have characteristic odors, suitable for perfumery.

IT 856607-18-6, 1-Propen-1-ol 3-bromo-, 3-(p-methoxyphenyl)-, acetate (preparation of)

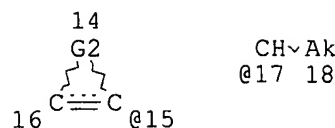
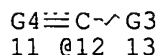
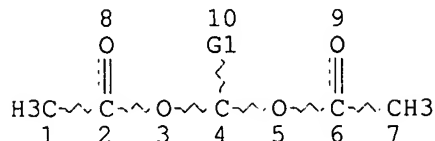
RN 856607-18-6 HCAPLUS

CN 1-Propen-1-ol 3-bromo-, 3-(p-methoxyphenyl)-, acetate (7CI) (CA INDEX NAME)



=&gt; d que stat l13

L5 STR



Ak @19

VAR G1=12/15

REP G2=(1-10) A

VAR G3=H/19

VAR G4=CH2/17

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 18

CONNECT IS E1 RC AT 19

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

L8 813 SEA FILE=REGISTRY SSS FUL L5

L13 486 SEA FILE=HCAPLUS ABB=ON L8(L) RACT+ALL/RL

=&gt; d ibib abs hitstr l13 477-486

L13 ANSWER 477 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:527037 HCAPLUS

DOCUMENT NUMBER: 73:127037

TITLE: Enzyme-catalyzed reactions between some 2-substituted 5-nitrofuran derivatives and glutathione

AUTHOR(S): Boyland, Eric; Speyer, B. E.

CORPORATE SOURCE: Chester Beatty Res. Inst., Roy. Cancer Hosp., London, UK

SOURCE: Biochemical Journal (1970), 119(3), 463-72

CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: English

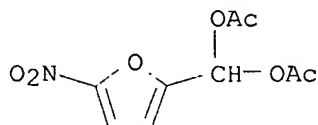
AB A glutathione transferase present in rat and human liver supernatant catalyzes the reaction of some 2-substituted 5-nitrofuran derivs. with GSH, with formation of a conjugate and release of the nitro group as inorg. nitrite. Some of the substrates undergo the same reaction at a slower rate in the absence of enzyme. Nitrofuran derivs. commonly used as drugs, and 5 other drugs containing nitro groups, did not react. Substrate activity in the nitrofuran derivs. showed an approx. correlation with the lability of the nitro group to alkali. Optimum pH values ranging from 6.6 to 9.0 were found for the enzymic reaction with various derivs., the values being influenced by alkali-lability and pK values of the compds. Tenfold purification of rat liver glutathione S-aryltransferase resulted in an equal purification of the activities that catalyze the reaction of 2 of the nitrofuran derivs. with GSH.

IT 92-55-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with glutathione in enzyme presence)

RN 92-55-7 HCAPLUS  
 CN Methanediol, (5-nitro-2-furanyl)-, diacetate (ester) (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 478 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1970:465651 HCAPLUS  
 DOCUMENT NUMBER: 73:65651  
 TITLE: Evidence for a cyclic AA1 1 mechanism in the hydrolysis of benzylidene diacetates  
 AUTHOR(S): Gregory, M. J.  
 CORPORATE SOURCE: Edward Chem. Lab., Aberystwyth, UK  
 SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), (6), 1201-7  
 CODEN: JCSPAC; ISSN: 0045-6470  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

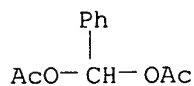
AB The acid-catalyzed hydrolyses of benzylidene diacetates were studied. The rates of hydrolyses depend on the Hammett acidity function  $H_0$ , and plots of  $\log K_{obs} + H_0$  against  $\log a_w$  had neg. slopes. The hydrolyses occur by an A1 mechanism, and the correlation of the rates of reaction with  $\sigma^+$  establishes that the mechanism is AA11. The entropies of activation obtained are consistent with the formation of a cyclic transition state, in which a protonated acetoxy group acts as a Lewis acid in assisting the loss of the second acetoxy group. p-Nitrobenzylidene diacetate appears to hydrolyze by the above mechanism at high acid concns. and by an AA2 mechanism at lower acidities. Only p-methoxybenzylidene diacetate showed an appreciably uncatalyzed reaction at 25°, and this reaction occurs by an  $SN_1$  type of process which also appears to involve a cyclic mechanism.

IT 581-55-5 2929-91-1 2929-93-3  
 13086-93-6 14202-31-4

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of, mechanism of)

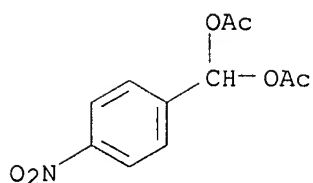
RN 581-55-5 HCAPLUS

CN Methanediol, phenyl-, diacetate (9CI) (CA INDEX NAME)

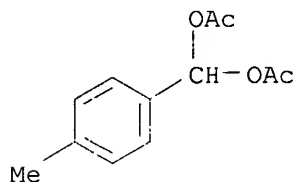


RN 2929-91-1 HCAPLUS

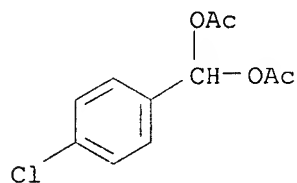
CN Methanediol, (4-nitrophenyl)-, diacetate (ester) (9CI) (CA INDEX NAME)



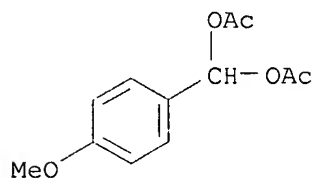
RN 2929-93-3 HCAPLUS  
CN Methanediol, (4-methylphenyl)-, diacetate (9CI) (CA INDEX NAME)



RN 13086-93-6 HCAPLUS  
CN Methanediol, (4-chlorophenyl)-, diacetate (9CI) (CA INDEX NAME)



RN 14202-31-4 HCAPLUS  
CN Methanediol, (4-methoxyphenyl)-, diacetate (9CI) (CA INDEX NAME)



L13 ANSWER 479 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1970:455322 HCAPLUS  
DOCUMENT NUMBER: 73:55322  
TITLE: Kinetics of alkaline hydrolysis of esters. III. Acyl acetals  
AUTHOR(S): Sharma, Raghunathprasad Chhitoram; Sharma, Man Moham  
CORPORATE SOURCE: Dep. Chem. Technol., Univ. Bombay, Bombay, India  
SOURCE: Bulletin of the Chemical Society of Japan (1970), 43(5), 1282-6  
CODEN: BCSJA8; ISSN: 0009-2673  
DOCUMENT TYPE: Journal



LANGUAGE: English

AB The kinetics of the alkaline hydrolysis of acyl acetals (liquid and solid) was studied in 90 parts (weight/weight) aqueous ethanol. Steric and inductive effects

played an important role. A straight line relation was observed between the rate consts. for the alkaline hydrolysis of benzylidene-, and m- and p-nitrobenzylidene diacetates and Hammett  $\sigma$  constant. In the case of butylidene and benzylidene diacetates, the theory of mass transfer accompanied by fast pseudo first-order reaction was employed for the

determination

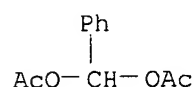
of rate constant in an aqueous medium.

IT 581-55-5 2929-91-1 6345-63-7  
29949-19-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of, mechanism of)

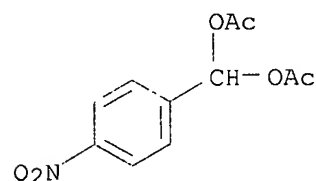
RN 581-55-5 HCAPLUS

CN Methanediol, phenyl-, diacetate (9CI) (CA INDEX NAME)



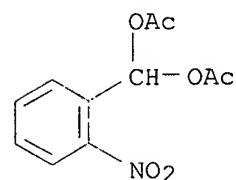
RN 2929-91-1 HCAPLUS

CN Methanediol, (4-nitrophenyl)-, diacetate (ester) (9CI) (CA INDEX NAME)



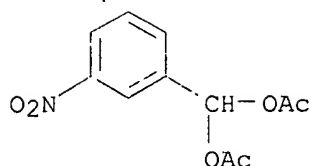
RN 6345-63-7 HCAPLUS

CN Methanediol, (2-nitrophenyl)-, diacetate (ester) (9CI) (CA INDEX NAME)

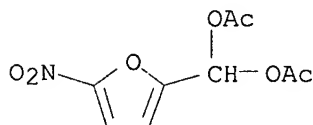


RN 29949-19-7 HCAPLUS

CN Methanediol, (3-nitrophenyl)-, diacetate (ester) (9CI) (CA INDEX NAME)



L13 ANSWER 480 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1970:54486 HCAPLUS  
 DOCUMENT NUMBER: 72:54486  
 TITLE: Solvatochromism of some derivatives of  $\alpha$ -nitrofurans and their reactivity during catalytic hydrogenation  
 AUTHOR(S): Reutov, G. A.; Finkel'shtein, A. V.; Reutova, E. A.  
 CORPORATE SOURCE: Sib. Tekhnol. Inst., Krasnoyarsk, USSR  
 SOURCE: Zhurnal Vsesoyuznogo Khimicheskogo Obshchestva im. D. I. Mendeleeva (1969), 14(5), 586-7  
 CODEN: ZVKOA6; ISSN: 0373-0247  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB 5-Substituted-2-nitrofurans were hydrogenated in MeOH at 30° under constant pressure of H in catalytic contact with Al<sub>2</sub>O<sub>3</sub> and a reduced Pd suspension; all reacted with zero order kinetics with respect to the substrate and the rate consts. ( $k + 103$  millimole/min) were as follows (5-substituent shown): CO<sub>2</sub>CH<sub>2</sub>Ph 87; CO<sub>2</sub>Et 81; CO<sub>2</sub>Me 79; CH(OAc)<sub>2</sub> 64; CH<sub>2</sub>OAc, 55; H, 45; CONHPh, 46; CHO, 33; CH<sub>2</sub>OH 33. The absorption spectra of the starting materials were reported. Thus the use of the equation suggested by Finkelshtein, et al., (1964) for calcn. of rate consts. of reactions from solvatochromic shifts in electronic absorption bands was applied to furan derivs. The equation takes the form  $\log k = -0.95 - 0.32 \cdot 10^{-3} \Delta \nu_{1,2}$ , the shift being determined in spectra taken in heptane and EtOH.  
 IT 92-55-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrogenation of, kinetics of)  
 RN 92-55-7 HCAPLUS  
 CN Methanediol, (5-nitro-2-furanyl)-, diacetate (ester) (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 481 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1969:448938 HCAPLUS  
 DOCUMENT NUMBER: 71:48938  
 TITLE: Absorption spectra and reactivity of some heterocyclic compounds. II. Temperature effect on the correlation between the values of the solvatochromic effect and the hydrogenation rate constants of 2-nitrofuran derivatives  
 AUTHOR(S): Finkel'shtein, A. V.; Reutov, G. A.

CORPORATE SOURCE: Sib. Tekhnol. Inst., Krasnoyarsk, USSR  
 SOURCE: Reaktsionnaya Sposobnost Organicheskikh Soedinenii  
 (1968), 5(4), 909-19  
 CODEN: RSOTAY; ISSN: 0375-9520

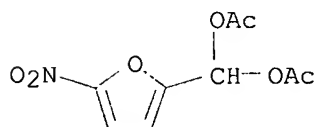
DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB The rate consts.,  $k$ , were determined for the hydrogenation of 5-substituted 2-nitrofuran derivs., the substituents being  $\text{CH}_2\text{OH}$ ,  $\text{CHO}$ ,  $\text{CONH}_2$ ,  $\text{PhNHCO}$ ,  $\text{MeCO}_2\text{CH}_2$ ,  $(\text{MeCO}_2)_2\text{CH}$ , and  $\text{BzO}$ . The hydrogenation was carried out in  $\text{MeOH}$  at 298, 303, 308, 313, and  $318^\circ\text{K}$ . Pd metal deposited on  $\text{Al}_2\text{O}_3$  was the catalyst. A linear dependence of  $\log k$  on the solvatochromic effect was found, sep. lines being formed for single reaction temps. In the equation  $\log k = a + b\Delta\epsilon_{1,2}$ , the temperature dependence of the coeffs.  $a$  and  $b$  is expressed as  $a = B_0 - (E_0/2.303RT)$  and  $b = C_1 - (C_2/T)$ , where the consts. have the following values:  $B_0 = 7.74$ ,  $E_0/2.303R = 2770$ ,  $C_1 = -0.00749$ , and  $C_2 = -0.16$ .

IT 92-55-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrogenation of, kinetics of)

RN 92-55-7 HCAPLUS

CN Methanediol, (5-nitro-2-furanyl)-, diacetate (ester) (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 482 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:36827 HCAPLUS

DOCUMENT NUMBER: 70:36827

TITLE: Absorption spectra and reactivity of some heterocyclic compounds. I. Hydrogenation of nitrofuran derivatives on palladium black

AUTHOR(S): Finkel'shtein, A. V.; Reutov, G. A.

CORPORATE SOURCE: Sib. Tekhnol. Inst., Krasnoyarsk, USSR

SOURCE: Reaktsionnaya Sposobnost Organicheskikh Soedinenii  
 (1968), 5(2), 341-9  
 CODEN: RSOTAY; ISSN: 0375-9520

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB Various 5-substituted 2-nitrofurans (I) were hydrogenated in  $\text{MeOH}$  at  $293^\circ$  and at a H pressure of 105 newtons/m.<sup>2</sup> in an exptl. arrangement similar to that described earlier (A. V. Finkel'shtein and V. V. Ivanov, 1967) by using 40 mg. Pd black, 50 ml.  $\text{MeOH}$ , and 1 millimole I for each run (at these conditions the corresponding furylamines were the final products); from the values obtained, the hydrogenation rate consts. ( $k$ ) were calculated. For the same I the values of the solvatochromic shifts for the heptane-EtOH solvent system ( $\Delta\epsilon_{1,2}$ ) were determined (Finkel'shtein, 1966). The results are (R of the I concerned,  $k + 103$ , wave length of the absorption maximum in heptane, and  $\Delta\epsilon_{1,2}$  given):  $\text{CO}_2\text{CH}_2\text{Ph}$  50, 288, 360;  $\text{CO}_2\text{Et}$  47, 288, 420;  $\text{CO}_2\text{Me}$  44, 287, 480;  $\text{CO}_2\text{Ph}$  33, 289, 590;  $\text{CH}(\text{OAc})_2$  34, 288, 710;  $\text{CO}_2\text{H}$  26, 289, 930;  $\text{CH}_2\text{OAc}$  26, 293, 910;  $\text{CONHPh}$  20, 240, 1180;  $\text{CH}_2\text{Br}$  16, 297, 1310;  $\text{CHO}$  11, 292, 1570; and  $\text{CH}_2\text{OH}$  10 millimole/min., 295 nm.,  $1640\text{ cm}^{-1}$ . A math. treatment of the

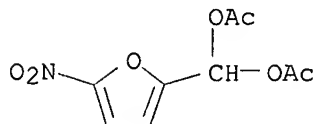
data gave the correlation  $\log k = -1.11 - (0.53 + 10^{-3})\Delta v_{1,2}$  characterized by a correlation coefficient = 0.996, a standard deviation = 0.02, and a Student criterion = 34.8.

IT 92-55-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of, kinetics of)

RN 92-55-7 HCAPLUS

CN Methanediol, (5-nitro-2-furanyl)-, diacetate (ester) (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 483 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:28121 HCAPLUS

DOCUMENT NUMBER: 70:28121

TITLE: Reactivity of ethylenic compounds: bromination.  
XXII. Quantitative evaluation of solvent effects  
(methanol, water) on  $\beta$ -heteropolar compounds

AUTHOR(S): Bienvenue-Goetz, E.; Dubois, Jacques E.

CORPORATE SOURCE: Fac. Sci., Paris, Fr.

SOURCE: Tetrahedron (1968), 24(23), 6777-89

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: German

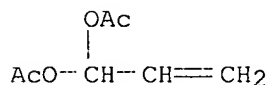
AB The investigation of several alkenes and  $\beta$ -heteropolar compounds covering a large range of reactivity (6.7 log units in water) leads to the homogeneous correlation  $\log k_{Br_2}[H_2O] = 1.08 \log k_{Br_2}[MeOH] + 4.3$ . This result shows that the structural effects are almost independent of the solvent effects in methanol and water. For certain substituents, in particular  $CH_2OH$  and  $CH(OAc)_2$ , large, specific "solvent-substituent" interactions are observed. Examination of parametric "reactivity/structure" correlations leads to attribution of these interactions to the solvent sensitivity of the polar effect. These phenomena are comparable with the behavior of substituted fluorobenzenes, expressed by means of 1H N. M. R chemical shifts.

IT 869-29-4, 2-Propene-1,1-diol, diacetate

RL: RCT (Reactant); RACT (Reactant or reagent)  
(bromination of, kinetics of)

RN 869-29-4 HCAPLUS

CN 2-Propene-1,1-diol, diacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



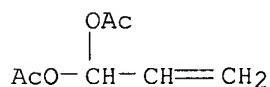
L13 ANSWER 484 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:466627 HCAPLUS

DOCUMENT NUMBER: 69:66627

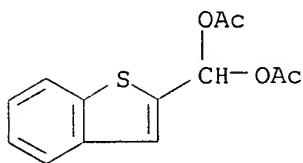
TITLE: Reactivity of ethylene compounds: bromination. XIX.  
Compatibility between experimental results and various

mechanistic hypotheses. Alkylated and  $\beta$ -heteropolar ethylenes  
 AUTHOR(S): Dubois, Jacques Emile; Bienvenue-Goetz, Elisabeth  
 CORPORATE SOURCE: Lab. Chim. Org. Phys., Fac. Sci. Paris, Paris, Fr.  
 SOURCE: Bulletin de la Societe Chimique de France (1968), (5),  
 2086-93  
 CODEN: BSCFAS; ISSN: 0037-8968  
 DOCUMENT TYPE: Journal  
 LANGUAGE: French  
 AB Bromination of  $\text{CH}_2:\text{CMeCH}_2\text{CH}(\text{OH})\text{Me}$ ,  $\text{trans-HOCH}_2\text{CH}:\text{CHCH}_2\text{OH}$ ,  $\text{CH}_2:\text{CHCH}_2\text{OH}$ ,  
 $\text{CH}_2:\text{CHCH}_2\text{Ph}$ ,  $\text{CH}_2:\text{CHCH}(\text{OH})\text{Bu}$ ,  $\text{CH}_2:\text{CHCH}(\text{OH})\text{Pr-iso}$ ,  $\text{CH}_2:\text{CHCH}_2\text{OPh}$ ,  
 $\text{CH}_2:\text{CHCH}_2\text{CO}_2\text{Me}$ ,  $\text{CH}_2:\text{CHCH}_2\text{Cl}$ ,  $\text{CH}_2:\text{CHCH}_2\text{CN}$ ,  $\text{CH}_2:\text{CHCH}(\text{CO}_2\text{Me})_2$ , and  
 $\text{trans-ClCH}_2\text{CH}:\text{CHCH}_2\text{Cl}$  was expressed by the equation  $\lg(1 + K[\text{Br-}]) =$   
 $\alpha + \beta[\text{Br-}]$ , where  $\lg$  was the rate constant,  $K$  the equilibrium constant  
 of the reaction  $\text{Br}_2 + \text{Br-} \rightarrow \text{Br}_3^-$  and  $\alpha$  and  $\beta$  are  
 interdependent consts. For reactive brominating agents  $\lg \alpha = \lg$   
 $\beta - 0.94$ , for less reactive ones  $\lg \alpha = 1.16 \lg \beta -$   
 1.86. 22 references.  
 IT 869-29-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (bromination of, mechanism of)  
 RN 869-29-4 HCAPLUS  
 CN 2-Propene-1,1-diol, diacetate (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 485 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1968:68250 HCAPLUS  
 DOCUMENT NUMBER: 68:68250  
 TITLE: Use of infrared and ultraviolet spectroscopy for  
 determining the structure of isomeric nitro compounds  
 in the thionaphthene series  
 AUTHOR(S): Mamaev, V. P.; Shkurko, O. P.  
 SOURCE: Primen. Mol. Spektrosk. Khim., Sb. Dokl. Sib.  
 Soveshch. Spektrosk., 3rd (1966), Meeting Date 1964,  
 45-6  
 CODEN: 16KMAD  
 DOCUMENT TYPE: Conference  
 LANGUAGE: Russian  
 AB The reaction mixture obtained on nitrating thionaphthene-2-carboxaldehyde  
 diacetate was analyzed by uv and ir spectroscopy. The uv anal. is based  
 on the fact that the nitrothionaphthene spectra are not affected by  
 introducing the methylene diacetate group. The 3-, 4-, and  
 5-nitrothionaphthene-2-carboxaldehydes were found in the ratio  
 3.5:4.0:2.5. On nitrating thionaphthene-2-carboxaldehyde in  $\text{Ac}_2\text{O}$ , the  
 isomers were found in the ratio 1.0:6.6:2.4. The nitration of  
 2-nitrovinylthionaphthene leads to a single product. The structure was  
 determined by oxidation to 4-nitrothionaphthene-2-carboxaldehyde. The  
 structures  
 of the products were confirmed by comparing the K bands in the uv spectra  
 with those of the corresponding styrenes.  
 IT 4565-35-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (nitration of, spectra in relation to)  
 RN 4565-35-9 HCAPLUS

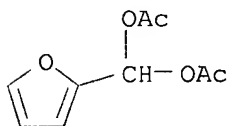
CN Benzo[b]thiophene-2-methanediol, diacetate (7CI, 8CI) (CA INDEX NAME)



L13 ANSWER 486 OF 486 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1967:411428 HCAPLUS  
 DOCUMENT NUMBER: 67:11428  
 TITLE: 5-Nitrofurfural diacetate  
 INVENTOR(S): Montague, Alexander P.  
 PATENT ASSIGNEE(S): Montague, Cecil S.  
 SOURCE: Brit., 2 pp.  
 CODEN: BRXXAA  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1061799		19670315	GB 1964-44104	19641029

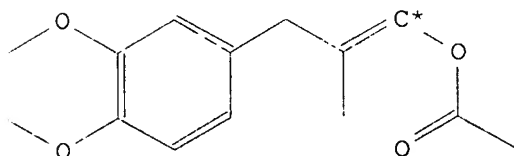
GI For diagram(s), see printed CA Issue.  
 AB The title compound (I) is prepared by nitration of furfural diacetate in concentrated H<sub>2</sub>SO<sub>4</sub>. Thus, an intimate mixture of 20 g. furfural diacetate, and 11.2 g. KNO<sub>3</sub> is gradually added to well-stirred and cooled concentrated H<sub>2</sub>SO<sub>4</sub> in a N atmospheric at such a rate that a temperature of -5 to 0° is maintained. When the addition is completed stirring is continued for 15 min. and 100 g. ice added followed by sufficient Na<sub>3</sub>PO<sub>4</sub>·12H<sub>2</sub>O to raised the pH to 3.5. The organic layer is separated, treated with 150 cc. ice-water, and extracted with ether to give after distillation I in 74% yield.  
 IT 613-75-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (nitration of)  
 RN 613-75-2 HCAPLUS  
 CN Methanediol, 2-furanyl-, diacetate (9CI) (CA INDEX NAME)



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L20 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6700126  
 Chemical Name (CN): acetic acid 3-(3,4-dimethoxy-phenyl)-2-methyl-propenyl ester  
 Autonom Name (AUN): acetic acid 3-(3,4-dimethoxy-phenyl)-2-methyl-propenyl ester  
 Molec. Formula (MF): C14 H18 O4  
 Molecular Weight (MW): 250.29  
 Lawson Number (LN): 6490, 1155, 289  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 2314706  
 Tautomer ID (TAUTID): 6373824  
 Beilstein Citation (BSO): 5-06  
 Entry Date (DED): 1994/07/15  
 Update Date (DUPD): 1994/07/22



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
BP	Boiling Point	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

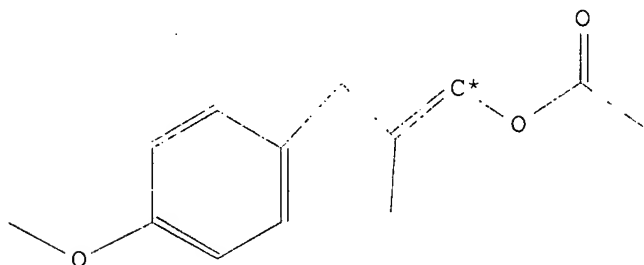
Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

All References:  
ALLREF

1. Scriabine, I., Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1961>, 1194-1198

L20 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2528663  
 Beilstein Pref. RN (BPR): 77104-98-4  
 CAS Reg. No. (RN): 77104-98-4  
 Chemical Name (CN): acetic acid 3-(4-methoxy-phenyl)-2-methyl-propenyl ester  
 Autonom Name (AUN): acetic acid 3-(4-methoxy-phenyl)-2-methyl-propenyl ester  
 Molec. Formula (MF): C13 H16 O3  
 Molecular Weight (MW): 220.27  
 Lawson Number (LN): 6033, 1155, 289  
 Compound Type (CTYPE): isocyclic  
 Constitution ID (CONSID): 2298036  
 Tautomer ID (TAUTID): 2447900  
 Beilstein Citation (BSO): 5-06  
 Entry Date (DED): 1989/07/05  
 Update Date (DUPD): 1994/07/22



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
BP	Boiling Point	1
RI	Refractive Index	1



This substance also occurs in Reaction Documents:

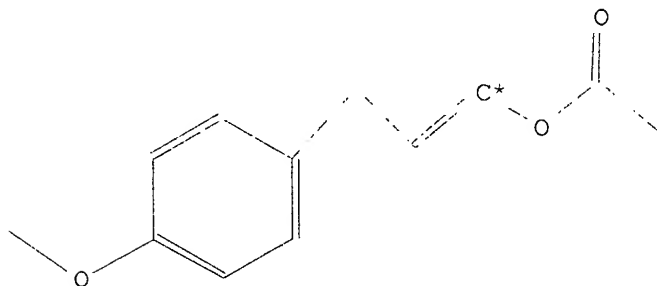
Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

All References:  
ALLREF

1. Scriabine, I., Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1961>, 1194-1198

L20 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2523870  
Beilstein Pref. RN (BPR): 91496-96-7  
CAS Reg. No. (RN): 91496-96-7  
Chemical Name (CN): acetic acid 3-(4-methoxy-phenyl)-propenyl ester  
Autonom Name (AUN): acetic acid 3-(4-methoxy-phenyl)-propenyl ester  
Molec. Formula (MF): C12 H14 O3  
Molecular Weight (MW): 206.24  
Lawson Number (LN): 6031, 1155, 289  
Compound Type (CTYPE): isocyclic  
Constitution ID (CONSID): 1926275  
Tautomer ID (TAUTID): 2440794  
Beilstein Citation (BSO): 5-06  
Entry Date (DED): 1989/07/05  
Update Date (DUPD): 1994/07/22



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1

LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
BP	Boiling Point	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

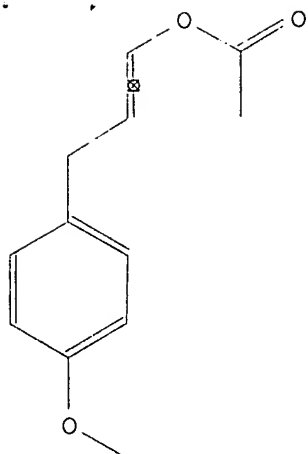
All References:

ALLREF

1. Scriabine, I., Bull.Soc.Chim.Fr., CODEN: BSCFAS, <1961>, 1194-1198

L20 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	2100019
Beilstein Pref. RN (BPR):	91496-96-7
CAS Reg. No. (RN):	91496-96-7
Chemical Name (CN):	acetic acid 3-(4-methoxy-phenyl)-propenyl ester
Autonom Name (AUN):	acetic acid 3-(4-methoxy-phenyl)-propenyl ester
Molec. Formula (MF):	C12 H14 O3
Molecular Weight (MW):	206.24
Lawson Number (LN):	6031, 1155, 289
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	1926275
Tautomer ID (TAUTID):	2038380
Beilstein Citation (BSO):	5-06
Entry Date (DED):	1989/06/29
Update Date (DUPD):	1989/07/12



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
BP	Boiling Point	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:  
ALLREF

1. Patent: Rhone-Poulenc DE 1145161 1963, Chem.Abstr., 59(9900d), <1963>